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Perturbation Theory for Shape Resonances and Large Barrier Potentials

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Abstract. We develop a systematic perturbation and resonance theory for the one-dimensional Schrödinger equation of the form

$$(-d^2/dx^2 + U(x) + \lambda V(x) - E)\psi(x) = 0, \quad 0 \leqq x < \infty,$$

where the barrier potential $V(x)$ is supported only where $x \geqq 1$ and is non-negative there, and λ is a real parameter tending to infinity. We prove that every $\lambda = \infty$ eigenvalue turns into a resonance or an eigenvalue for finite λ.

1. Introduction

One of the standard problems treated in elementary quantum mechanics textbooks is the decay of a nucleus via alpha emission. The discussion is customarily based on a simplified model wherein the alpha particle is acted upon by a spherically symmetric potential comprising a short-range negative piece from the attraction between nucleons and a long-range repulsive piece from the electric interaction between protons. The large potential barrier has two effects, viz., that it confines the alpha particle for long periods until it escapes by tunneling, and that it alters the energy levels of the bound or quasi-bound states. A representative discussion is to be found in [1].

This paper addresses the two principal mathematical problems connected with this model:

1. To develop a perturbation series for the bound states and resonance energies in the limit as the barrier size is elevated to infinity. This does not appear to have been done systematically before, probably owing to the very singular sort of limit as $\lambda \to \infty$. It will turn out that the series involves fractional powers of $1/\lambda$, λ being the variable parametrizing the height of the barrier; in particular, when $V(x) \sim$

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$(x-1)^p$ as $x \downarrow 0$, $p \geqq 0$, the fractional power is $\lambda^{-1/(p+2)}$. Moreover, the series is sensitive only to the inner edge of the barrier, for which reason it can not generally converge to the correct value for finite λ, but is valid in the usual asymptotic sense of perturbation theory. We therefore also derive formulae for the exponentially small effect of varying the interior of the barrier (at $x \geqq 1+\varepsilon$) on the eigenvalues.

2. To evaluate the exponentially small resonance widths, which we regard simply as (proportional to) the imaginary parts of resonance eigenvalues as defined with Gamow–Siegert boundary conditions outside the barrier. See [2] for a discussion of the connection between this point of view and those involving poles of the S-matrix or time-dependent quantities. A rather extensive literature already exists on this second problem and can be traced through quantum-mechanics textbooks [1, 3]. We would like, however, to call attention to the recent work of N. Fröman et al. [4], whose highly developed variation-of-parameters techniques have been used to analyze the resonances, considered as zeroes of the Jost function, in the case of analytic barrier potentials. Their situation does not involve the limit $\lambda \to \infty$, and they discuss tunneling near the top of the barrier, which will not be attempted here. Their formulae would agree with some of ours in the appropriate limit. Related ideas have been used to study resonances in the Stark effect [5], where there are, however, several important technical differences (and additional complications).

The discussion below will be in the language of ordinary differential equations and perturbation theory. Though it would seem to apply only to the case of spherical symmetry in the n-dimensional case, it is clear that asymmetries in the region $r > 1+\varepsilon$ affect very little, because upper and lower bounds for the eigenvalue perturbations are obtainable from the min-max principle by comparison with spherically symmetric potentials that have been maximized or minimized in the angular variables for each value of r, and the spherically symmetric comparison operators have identical perturbation series (see below). Moreover, as has been stressed by Lavine [6], decay rates of resonances can be estimated above and below by comparison with angularly maximized and minimized problems.

Hence, from the outset we shall consider the ordinary differential operator

$$H(\lambda) = -d^2/dx^2 + U(x) + \lambda V(x) \quad \text{on } L^2(\mathbb{R}^+), \tag{1.1}$$

where U is supported in $[0, 1]$ and continuous except for a finite number of finite jump discontinuities. Also $\lim\limits_{x\downarrow 0} x^2 u(x) = \ell(\ell+1)$, $\ell = 0, 1, 2, \ldots$. We assume V, supported in $[1, \infty)$, is C^2 except for a finite number of finite jump discontinuities and satisfies conditions appropriate for either 1) the bound-state problem, or 2) the resonance problem, i.e.:

1) $\operatorname{supp}(V) = [1, \infty)$ and $V \geqq b > 0$ on $[1, \infty)$,

except possibly in a neighborhood of $x = 1$, where $V'(x) > 0$, $V(1) = 0$ is allowed, and, as technical hypotheses we shall require that $V(x)e^{-\varepsilon x}$ is bounded for some $\varepsilon > 0$ and that

$$\int_x^\infty \left| (V(x)-E)^{-1/4} \frac{d^2}{dx^2} (V(x)-E)^{-1/4} \right| dx \tag{1.2}$$

is finite for $1 \leqq x$ and all $E \leqq 0$; or

2) $\mathrm{Supp}(V) = [1, a]$ for some $a < \infty$, and $V > 0$ on $(1, a)$.
It should not be difficult to extend case (2) to cover tails of V extending to infinity, either scaled with λ or not, except that the connections among the various notions of resonance become less clear. It also becomes more laborious to work with the resonance condition: a resonance state becomes asymptotic to

$$(E - \lambda V)^{-1/4} \exp(i \int^x \sqrt{E - \lambda V} dx)$$

as $x \to \infty$ (or something worse if V does not fall off nicely enough), which leads to λ-dependent ranges in x and more complicated asymptotic estimates.

The problem to be perturbed about has λ formally infinite, so it will be supposed that the solution y_0 of

$$(-d^2/dx^2 + U(x) - E)y_0(x) = 0, \quad 0 \leqq x \leqq 1, \tag{1.3}$$

with Dirichlet boundary conditions at $x = 0$ is known for a range of E. Its normalization can be fixed so that it is an entire function of E[7, 8]. Observe that the domain of definition of (1.1) suffers a sudden contraction at $\lambda = \infty$, and that as $\lambda \to \infty$ the eigenvalues $E(\lambda)$ ought to approach the eigenvalues e of (1.3) with the additional requirement that $y_0(1) = 0$ (indices on eigenvalues will be dropped whenever no confusion can result). We prove this fact below. The way to cope with the sudden domain change will be to identify a modified "unperturbed" problem containing the dominant effect of the V and having computable asymptotics.

The following section will define the eigenvalues and other objects of interest, and will prove that eigenvalues and resonances converge properly and have power series sensitive only to values of V in an arbitrarily small neighborhood of $x = 1$. The exponentially small differences due to the interior of the barrier and the resonance widths from tunneling will be estimated. An important consequence of this is that it enables a modified problem, which contains part of the perturbation but can be analyzed by hand, to be identified. The modified problem controls the form of the perturbation series and the leading term. Then a careful analysis of the spectral projection operators yields the perturbation series in inverse fractional powers of the barrier height; the term formally similar to ordinary first-order perturbation theory will only show up at the second lowest order.

2. Definitions, Convergence, and the Exponentially Small Effect of the Interior of the Barrier

In the language of ordinary differential equations, eigenvalues and resonances will be considered as determined by linear dependence of solutions. The definitions are equivalent to those by square-integrability and "purely outgoing exterior waves." Let ψ, variously subscripted, denote a solution of

$$(-d^2/dx^2 + U(x) + \lambda V(x) - E)\psi(x) = 0. \tag{2.1}$$

The solution with Dirichlet boundary conditions (or, respectively, Dirichlet-like conditions, that it is $\sim x^{\ell}$) at $x = 0$ will be denoted ψ_0; clearly, for $0 \leqq x \leqq 1$, $\psi_0 = y_0$. For bound states (case (1) or case (2) with $E < 0$), ψ_∞ denotes the subdominant solution, normalized so that

$$\psi_\infty(x)/((\lambda V(x)-E)^{-1/4}\exp(-\int_1^x(\lambda V(x')-E)^{1/2}dx')\to 1 \text{ as } x\to\infty, \tag{2.2}$$

and for resonances (case (2) with Re$E>0$*),* Ψ_∞ *denotes the outgoing solution* defined by $\psi_\infty(a)=1, \psi'_\infty(a)=i\sqrt{E}$. (Our convention is that the branch cut for $z^{1/2}$ is on the negative real axis.)

Definition 2.1. An eigenvalue of (1.1) is a real solution $E(\lambda)$ of the implicit equation

$$0=F(E,\lambda)\equiv\frac{\psi_0(1;E,\lambda)}{\psi'_0(1;E,\lambda)}-\frac{\psi_\infty(1;E,\lambda)}{\psi'_\infty(1;E,\lambda)}=\frac{W\{\psi_0,\psi_\infty\}}{\psi'_0(1)\psi'_\infty(1)}, \tag{2.3}$$

for case (1) or case (2) with $E<0$. A resonance of (1.1) is a complex solution of the same equation with ψ_∞ defined as for resonances. The parameter λ is allowed to assume the value ∞, in which case $\psi_\infty/\psi'_\infty|_{x=1}$ is interpreted as 0. (Prime means $\frac{d}{dx}$, and the parameters E and λ will often be suppressed below.)

Remark. It is of course conceivable that the denominators in (2.3) vanish, in which case the conditions are replaced with the conditions that $\psi'_0/\psi_0-\psi'_\infty/\psi_\infty=0$. In the limit we consider, however, only the numerators vanish (approximate Dirichlet conditions at $x=1$, c.f. the pointwise estimates (2.6) – (2.11)).

Lemma 2.2. *For any sufficiently large, fixed* $\lambda\leqq\infty$, *there is a complex neighborhood in* E *of any unperturbed eigenvalue, on which* $F(E,\lambda)$ *is analytic in* E.

Remark. The domain of analyticity is restricted only by the possible vanishing of the denominator.

Proof. This is more or less standard; in [7, 9] (see also [10] for a streamlined proof and [23] for related material) it is shown that the solutions of (2.1) and their derivatives are analytic in E at any fixed x, when there is a boundary condition fixing them at some point x_0, or making them depend analytically on E at x_0. This proves the Lemma for resonances, which have boundary conditions only at finite points. (Resonances at 0, if 0 is an eigenvalue at $\lambda=\infty$, are not considered.) The case involving subdominancy is essentially equivalent to the well-known fact [9, 23] that the Green function

$$G(x,x',E)=\psi_0(x_<)\psi_\infty(x_>)/W\{\psi_0,\psi_\infty\}, \tag{2.4}$$

where $x_<$ and $x_>$ are the lesser and greater of x and x', is analytic except at the spectrum of (1.1), having simple poles for $E<\liminf_{x\to\infty}\lambda V(x)$ at the eigenvalues, coming only from the zeroes of the Wronskian. Since

$$1/G(1,1,E)=\psi'_\infty(1;E,\lambda)/\psi_\infty(1;E,\lambda)-\psi'_0(1;E,\lambda)/\psi_0(1;E,\lambda),$$

and we already know the analyticity of ψ'_0 and ψ_0, this establishes the analyticity of $\psi_\infty/\psi'_\infty(1;E,\lambda)$, except at zeroes of ψ'_∞. For λ large enough, these zeroes will not occur, because ψ'_∞ is strictly decreasing in absolute value on the largest interval $[x_0, \infty)$ on which $V - E > 0$ [11]. (If $V(1) = 0$, and $\lim_{x \downarrow 1} V'(x) > 0$, then this fact does not suffice to eliminate the zeroes, and we instead appeal to the asymptotic estimate (2.7) below.) □

We next collect some fairly standard pointwise asymptotic estimates for ψ_∞. Suppose first that case (1) applies and that $V(1) > 0$. Then because of the scaling with λ and the assumptions on (1.2),

$$\int_x^\infty \left|(\lambda V(x) - E)^{-1/4} \frac{d^2}{dx^2}(\lambda V(x) - E)^{-1/4}\right| dx \tag{2.5}$$

is $O(\lambda^{-1/2})$ uniformly for all negative E and $x \geqq 1$. This ensures [12] that WKB approximations are valid in the sense that, uniformly in $x \geqq 1$ and for $E \leqq 0$,

$$\psi_\infty(x) = (\lambda V(x) - E)^{-1/4} \exp\left(-\int_1^x \sqrt{\lambda V(x') - E}\, dx'\right) \cdot (1 + O(\lambda^{-1/2})), \tag{2.6a}$$

and this formula remains valid when differentiated:

$$\psi'_\infty(x) = -(\lambda V(x) - E)^{+1/4} \exp\left(-\int_1^x \sqrt{\lambda V(x') - E}\, dx'\right) \cdot \left(1 + O(\lambda^{-1/2})\right). \tag{2.6b}$$

In case (1) with $V(1) = 0$, $\lim_{x \downarrow 1} V'(x) > 0$, if E is real or nearly so, then Eqs. (2.6) are valid only on the interval $[1 + \lambda^{-1/3+\alpha}, \infty)$, $0 < \alpha < 1/3$, with multiplicative errors $1 + O(\lambda^{-3\alpha/2})$, by a computation of (2.5). For $1 \leqq x \leqq \lambda^{-1/3+\alpha} + 1$ one must use Langer's uniform approximation,

$$\begin{aligned} \psi_\infty(x) &= \text{const}\, Ai\left(\left(\frac{3}{2} \int_{1+E/\lambda V'(1)}^x \sqrt{\lambda V(x') - E}\, dx'\right)^{2/3}\right) \cdot (1 + O(\lambda^{-1/3+3\alpha/2})), \\ \psi'_\infty(x) &= \text{const}\, \frac{d}{dx} Ai\left(\left(\frac{3}{2} \int_{1+E/\lambda V'(1)}^x \sqrt{\lambda V(x') - E}\, dx'\right)^{2/3}\right) \cdot (1 + O(\lambda^{-1/3+3\alpha/2})) \end{aligned} \tag{2.7}$$

[13, 14, 15]. Clearly, α must be chosen between 0 and 2/9 for the interval of validity to overlap, though as usual the exact value of α will be irrelevant to any actual computations.

Remark. Early references to Langer's approximation make somewhat too restrictive assumptions, while later ones to this popular method have a disturbing tendency to ignore conditions for its validity. However, a slight modification of the variation-of-parameters argument of [5, 16] shows that (2.7) depends on knowing that

$$\int_1^{1+\lambda^{-1/3+\alpha}} \left| \frac{B(x; \lambda, E)\, a(x; \lambda, E)\, b(x; \lambda, E)}{W\{a(x; \lambda, E), b(x; \lambda, E)\}} \right| dx = O(\lambda^{-1/3+3\alpha/2}), \tag{2.8}$$

where a and b are respectively Ai and Bi with the arguments

$$\left(\frac{3}{2} \int_{1+E/\lambda V'(1)}^x \sqrt{\lambda V(x') - E}\, dx'\right)^{2/3},$$

and B is defined by

$$\left(-\frac{d^2}{dx^2}+\lambda V-E\right)a(x)=B(x)\,a(x).$$

Though B is somewhat unpleasant, it is straightforward to show (2.8) with the asymptotics of Airy functions of [17] and some simple Taylor expansions. The constant in (2.7) can be read off from the known asymptotics of the Airy functions when ψ_∞ is required to be continuous at the matching point; it is $2\sqrt{\pi}(\lambda V'(1))^{-1/6}$.

In case (2), if $V(a)>0$, then the outer boundary condition implies

$$\psi_\infty(x)=\left[\left(\frac{\lambda V(a)-E}{\lambda V(x)-E}\right)^{1/4}\cosh\left(\int_x^a\sqrt{\lambda V(x')-E}\,dx'\right)-\frac{i\sqrt{E}\sinh\left(\int_x^a\sqrt{\lambda V(x')-E}\,dx'\right)}{((\lambda V(x)-E)(\lambda V(a)-E))^{1/4}}\right]\cdot(1+O(\lambda^{-1/2})),\tag{2.9}$$

and, as before this formula remains valid when differentiated (indeed, the second term is only relevant for ψ'_∞, and then only for x near a). If $V(a)=0$, $\lim_{x\uparrow a}V'(x)<0$, then the outer turning point must again be taken care of with Langer's approximation, which in this case says that for $x\in[a-\lambda^{-1/3+\alpha},a]$,

$$\psi_\infty(x)=\left[c\,Ai\left(\left(\frac{3}{2}\int_x^{a+E/\lambda V'(a)}\sqrt{\lambda V(x')-E}\,dx'\right)^{2/3}\right)+d\,Bi\left(\left(\frac{3}{2}\int_x^{a+E/\lambda V'(a)}\sqrt{\lambda V(x')-E}\,dx'\right)^{2/3}\right)\right]\cdot(1+O(\lambda^{-1/3+3\alpha/2})),\tag{2.10}$$

where

$$c=\pi(Bi'(0)-i\,Bi(0)\sqrt{E}/(\lambda V'(a))^{1/3})\to\frac{3^{1/6}\pi}{\Gamma(1/3)},$$

and

$$d=-\pi(Ai'(0)-i\,Ai(0)\sqrt{E}/(\lambda V'(a))^{1/3})\to\frac{\pi}{3^{1/3}\Gamma(1/3)}.$$

Formula (2.10) may be differentiated. In the rest of the barrier we then get

$$\psi_\infty(x)=\frac{(-\lambda V'(a))^{1/6}d}{\sqrt{\pi}}(\lambda V(x)-E)^{-1/4}\exp\left(\int_x^a\sqrt{\lambda V(x')-E}\,dx'\right)\cdot(1+O(\lambda^{-3\alpha/2})),$$

$$\psi'_\infty(x)=-\frac{(-\lambda V'(a))^{1/6}d}{\sqrt{\pi}}(\lambda V(x)-E)^{1/4}\exp\left(\int_x^a\sqrt{\lambda V(x')-E}\,dx'\right)\cdot(1+O(\lambda^{-3\alpha/2}))\tag{2.11}$$

(again with terms proportional to (2.7) near $x=1$). We shall not consider the cases where $V'(1)$ or $V'(a)=0$ as well, but note that everything is similar except that parabolic cylinder functions and the like appear.

These basic estimates will appear in several later applications. Less refined ones would have sufficed for the following:

Lemma 2.3. *$F(E,\lambda)$ and $\dfrac{\partial}{\partial E}F(E,\lambda)$ are continuous in λ as $\lambda\uparrow\infty$,*

and $\lim\limits_{\lambda\uparrow\infty} F(E,\lambda)=\dfrac{\psi_0(1;E,\lambda)}{\psi_0'(1;E,\lambda)}$ *and* $\lim\limits_{\lambda\uparrow\infty}\dfrac{\partial}{\partial E}F(E,\lambda)=\dfrac{\partial}{\partial E}\left(\dfrac{\psi_0(1;E,\lambda)}{\psi_0'(1;E,\lambda)}\right)$.

Proof. Since ψ_0 is independent of λ, this is equivalent to continuity of $\left(\dfrac{\psi_\infty}{\psi_\infty'}\right)$ and $\dfrac{\partial}{\partial E}\left(\dfrac{\psi_\infty}{\psi_\infty'}\right)$. The former fact is obvious from the estimates (2.6) – (2.11), which show that $\left.\dfrac{\psi_\infty}{\psi_\infty'}\right|_{x=1}\to 0$ in all cases. The latter fact follows from the formula

$$\frac{\partial}{\partial E}\left(\frac{\psi_\infty(x;E,\lambda)}{\psi_\infty'(x;E,\lambda)}\right)=\begin{cases}\dfrac{-\int_x^\infty\psi_\infty^2(x';E,\lambda)dx'}{(\psi_\infty'(x;E,\lambda))^2}, & \text{case (1)}\\[2ex] \dfrac{-\frac{i}{2}E^{-1/2}-\int_x^a\psi_\infty^2(x';E,\lambda)dx'}{(\psi_\infty'(x;E,\lambda))^2}, & \text{case (2).}\end{cases}\tag{2.12}$$

If $x=1$, formulae (2.6)–(2.11) and integration by parts show that $\dfrac{\partial}{\partial E}\left(\dfrac{\psi_\infty(1;E,\lambda)}{\psi_\infty'(1;E,\lambda)}\right)\to 0$ like a negative power of λ. The proof of (2.12) is that since $\dfrac{\psi_\infty}{\psi_\infty'}$ is differentiable in E and x, letting $v=\dfrac{\psi_\infty}{\psi_\infty'}$,

$$v_E'=v^2-2vv_E(\lambda V-E).$$

The solution of this is easily verified to be

$$v_E=\frac{\int^x\psi_\infty^2(x';E,\lambda)dx'}{(\psi_\infty'(x;E,\lambda))^2}.\tag{2.13}$$

Equation (2.12) is just this with the limits of integration chosen to satisfy the condition of subdominancy or respectively the boundary condition at a. $\square$

A corollary of Lemmas 2.2 and 2.3 with the implicit function theorem is that the eigenvalues and resonances are stable. The implicit function theorem is needed in the following form:

Theorem 2.4. *Let $F(E,\eta)$ and $\partial F(E,\eta)/\partial E$ be defined and continuous complex-valued functions of the variables $(E,\eta)\in\mathbb{C}\times\mathbb{R}^+$ in a neighborhood of $(E_0,0)$. Suppose that $F(E_0,0)=0$ and $\partial F(E_0,0)/\partial E\neq 0$. Then there exists an interval $[0,\varepsilon)$ for η and a unique function, denoted $E(\eta)$, continuous on $[0,\varepsilon)$, with $E(0)=E_0$, and such that $F(E(\eta),\eta)=0$ for all $\eta\in[0,\varepsilon)$. In case E and η are both complex variables and F is analytic in both of them at $(E_0,0)$, $E(\eta)$ becomes a unique analytic function of η in a complex neighborhood of 0.*

Remark. The analytic implicit function theorem can be found in [18]. The proof of the ordinary implicit function theorem in [19] makes no essential use of its assumption that the η neighborhood extends in both directions from 0, and its assumption of differentiability in η is used a) for the formula for implicit differentiation and b) to identify a small neighborhood in (E, η) on which $\partial F/\partial E$ is bounded away from zero. We shall not require the formula for implicit differentiation except in the analytic case, and continuity of $\partial F/\partial E$ suffices for b).

Corollary 2.5. *Given any $\lambda = \infty$ eigenvalue e, for λ large enough there is a unique eigenvalue or resonance $E(\lambda)$ in a complex neighborhood of e, converging to e as $\lambda \uparrow \infty$. $E(\lambda)$ is real for bound states. There are no finite accumulation points of solutions to $F(E, \lambda) = 0$ as $\lambda \uparrow \infty$ other than the $\lambda = \infty$ eigenvalues.*

Proof. Let η in the implicit function Theorem 2.4 be a negative power of λ, and abuse notation by letting $F(E, \eta)$ denote $F(E, \lambda)$. The assumptions of 2.4 (without analyticity) hold by 2.2 and 2.3, and because by definition if $E_0 = e$, then $F(E_0, \eta = 0) = 0$, and by (2.13) with ψ_0 replacing ψ_∞

$$\frac{\partial F(E_0, \eta = 0)}{\partial E} = (\psi_0'(1; E, \lambda))^{-2} \int_0^1 (\psi_0(x; E, \lambda))^2 dx > 0.$$

The reality of bound states follows from self-adjointness (and the non-zero imaginary parts of resonances are calculated explicitly below). Now consider E in a fixed, finite, complex neighborhood N. For λ very large, the estimates (2.6)–(2.11) hold uniformly on N (except that for Im E fixed different from 0 the Airy functions will not be needed when λ is large enough). The explicit formulae then show that $\psi_\infty(1; E, \lambda)/\psi_\infty'(1; E, \lambda) \to 0$ uniformly on N as $\lambda \uparrow \infty$. However, from the continuity of ψ_0/ψ_0' in E and the known spectrum of the $\lambda = \infty$ problem, $\psi_0/\psi_0' \geqq \varepsilon$ for some $\varepsilon > 0$ throughout N with some arbitrarily small neighborhoods of the e's removed. Thus eventually there can not be any extraneous solutions on N. □

Note. The referee has informed us that stability also follows from material in [24].

Before developing a systematic perturbation series, we shall show that it can only depend on V in an arbitrarily small neighborhood of $x = 1$ and estimate the (exponentially-small) effects due to the interior of the barrier. Suppose V_a and V_b agree for $1 \leqq x \leqq 1 + \varepsilon$, but may differ beyond that point, and let $E_a(\lambda)$ and $E_b(\lambda)$ denote eigenvalues or resonances with V_a and V_b respectively. Subscripting the eigenvalue conditions also with a and b, we then have

$$\begin{aligned}\delta(E, \lambda) \equiv F_a(E, \lambda) - F_b(E, \lambda) &= \psi_{\infty,b}/\psi'_{\infty,b}(1; E, \lambda) - \psi_{\infty,a}/\psi'_{\infty,a}(1; E, \lambda) \\ &= W\{\psi_{\infty,b}, \psi_{\infty,a}\}/\psi'_{\infty,b}(1; E, \lambda)\psi'_{\infty,a}(1; E, \lambda) \\ &= \frac{\psi'_{\infty,b}(1+\varepsilon; E, \lambda)\psi'_{\infty,a}(1+\varepsilon; E, \lambda)}{\psi'_{\infty,b}(1; E, \lambda)\psi'_{\infty,a}(1; E, \lambda)} \\ &\quad \cdot \left[\frac{\psi_{\infty,b}}{\psi'_{\infty,b}}(1+\varepsilon; E, \lambda) - \frac{\psi_{\infty,a}}{\psi'_{\infty,a}}(1+\varepsilon; E, \lambda)\right],\end{aligned} \tag{2.14}$$

since the Wronskian is constant for $1 \leqq x \leqq 1 + \varepsilon$.

Now, *this is an exponentially small function of λ uniformly for E confined to any compact set,* because of the exponential shrinking contained in the estimates-(2.6)–(2.11) and the consequence of the same estimates that the inverse logarithmic derivatives are bounded by a negative power of λ. Next, make a Taylor expansion in E for fixed λ, using the knowledge that $E_{a,b} \to e$:

$$\begin{aligned} 0 = F_a(E_a, \lambda) &= F_b(E_a, \lambda) + \delta(E_a, \lambda) \\ &= 0 + (E_a - E_b)\left(\frac{\partial F_b}{\partial E}(E_b, \lambda) + R(E_a, \lambda)\right) + \delta(E_a, \lambda), \end{aligned}$$

where by analyticity

$$\frac{R(E_a, \lambda)}{\dfrac{\partial F_b}{\partial E}(E_b, \lambda)} \to 0 \text{ as } E_a \to E_b$$

for any fixed λ, and the limit is uniform for λ^{-1} in the compact set $[0, \varepsilon]$, $\varepsilon > 0$, Therefore

$$(E_a - E_b) \sim \frac{-\delta(E_a, \lambda)}{\dfrac{\partial F_b}{\partial E}(E_b, \lambda)},$$

and (for case (1)), by (2.13) and its analogue with ψ_0,

$$\begin{aligned} \frac{\partial F_b}{\partial E}(E_b, \lambda) &= \frac{\int_0^1 \psi_0^2(x)dx}{(\psi_0'(1))^2} + \frac{\int_1^\infty \psi_{\infty,b}^2(x)dx}{(\psi_\infty'(1))^2} \\ &\to \frac{\int_0^1 y_0^2(x, e)dx}{(y_0'(1, e))^2} \end{aligned}$$

(and similarly for case (2)). By hypothesis this is a known, positive number, so we have proved:

Theorem 2.6. *For eigenvalues or resonances as defined above,*

$$E_a - E_b \sim \frac{-\delta(E_a, \lambda)(y_0'(1, e))^2}{\int_0^1 y_0^2(x, e)dx} = O(\lambda^{-n}),$$

for all $n < \infty$, where δ is given by (2.14).

Remark. The tilde means that the ratio approaches 1.

There is an alternative formula for the imaginary part of a resonance, which makes the problem of controlling real and imaginary errors separately in Theorem 6 somewhat easier:

Theorem 2.7. *Let E be a resonance; then its real part has the same Taylor series as any related problem such that $\tilde{V} \geqq C > 0$, but $\tilde{V}$ agrees with V on an arbitrarily* *small neighborhood* $[1, 1+\varepsilon]$. *The Taylor series coefficients are all real* (*if they exist*). *The imaginary part satisfies*

$$\operatorname{Im} E(\lambda) = \frac{\operatorname{Im} \bar{\psi}'(a)\psi(a)}{\int_0^a |\psi(x)|^2\,dx} \tag{2.15}$$

(*where* $\psi(x) \propto \psi_0(x; E(\lambda), \lambda) \propto \psi_\infty(x; E(\lambda), \lambda)$).

Remark. An analogous formula for the Stark effect has been used in [20].

Proof. We have already established that the Taylor series, in so far as they exist, are identical by Theorem 2.6, and reality follows from the self-adjointness of the problem with $\tilde{V}$. Equation (2.15) results from integrating

$$E(\lambda)\int_0^a |\psi(x)|^2\,dx = \int_0^a \bar{\psi}(x)\left(-\frac{d^2}{dx^2} + U + \lambda V\right)\psi(x)dx$$

by parts twice and solving for $\operatorname{Im} E(\lambda) = \dfrac{E(\lambda) - \bar{E}(\lambda)}{2i}$. □

The value a is special only in that $\operatorname{Im} \bar{\psi}'\psi$ is not dominated by the errors in $\bar{\psi}'\psi$ by (2.6)–(2.11) when $x = a$; if the integral ran only to some $x_0 < a$, then $\operatorname{Im} \bar{\psi}'\psi$ would be dominated by them. Noting that

$$\int_1^a \sqrt{\lambda V(x) - E}\,dx = \int_1^a \sqrt{\lambda V(x)}\,dx + 0(\lambda^{-1/2})$$

and using (2.6)–(2.11) in the various cases produces the following specific estimates:

Theorem 2.8. *If* $V(1)$ *and* $V(a)$ *are both positive, then*

$$\operatorname{Im} E(\lambda) \sim -\frac{4\sqrt{\operatorname{Re} E(\lambda)}\sqrt{V(1)}\,y_0^2(1, E(\lambda))\exp\left(-2\int_1^a \sqrt{\lambda V(x)}\,dx\right)}{\sqrt{V(a)}\int_0^1 y_0^2(x, e)\,dx}. \tag{2.16a}$$

If $V(1) > 0$, $V(a) = 0$, *and* $V'(a) \equiv \lim\limits_{x\uparrow a} V'(x) < 0$, *then*

$$\operatorname{Im} E(\lambda) \sim -\frac{3^{2/3}\Gamma^2(1/3)\sqrt{\operatorname{Re} E(\lambda)}\sqrt{V(1)}\,y_0^2(1, E(\lambda))}{\pi(-V'(a))^{1/3}\int_0^1 y_0^2(x, e)\,dx}\lambda^{1/6}\exp\left(-2\int_1^a \sqrt{\lambda V(x)}\,dx\right). \tag{2.16b}$$

If $V(1) = 0$, $V'(1) \equiv \lim\limits_{x\downarrow 1} V'(x) > 0$, *and* $V(a) > 0$, *then*

$$\operatorname{Im} E(\lambda) \sim -\frac{3^{4/3}\Gamma^2(2/3)\sqrt{e}\,y_0^2(1; E(\lambda))(V'(1))^{1/3}}{\pi\sqrt{V(a)}\int_0^1 y_0^2(x, e)\,dx}\lambda^{-1/6}\exp\left(-2\int_1^a \sqrt{\lambda V(x)}\,dx\right). \tag{2.16c}$$

If $V(1) = 0 = V(a)$, $V'(1) > 0$, *and* $V'(a) < 0$, *then*

$$\operatorname{Im} E(\lambda) \sim -\frac{3\sqrt{e}\,y_0^2(1;E(\lambda))}{\int_0^1 y_0^2(x,e)\,dx}\left(\frac{V'(1)}{-V'(a)}\right)^{1/3} \exp\left(-2\int_1^a \sqrt{\lambda V(x)}\,dx\right). \tag{2.16d}$$

3. The Perturbation Expansion

In this section we turn our attention to the development of an asymptotic series expansion in powers of $1/\lambda$ for $E(\lambda)$, where $E(\lambda)$ is an eigenvalue or resonance of $H(\lambda)$ as given in Definition 2.1. The information provided by Theorems 2.6 and 2.7 allows us to concentrate exclusively upon bound-state problems (case (1)) without loss of generality. Since in this case we are dealing with eigenvalues of a self-adjoint operator we are in a position to bring standard techniques and results from operator theory [21] to bear upon the problem.

As noted previously, the problem we address should be considered as a perturbed problem related to the $\lambda = \infty$ problem (1.3). However, these problems are too dissimilar for a direct approach using perturbation theory to be successful. To make progress, we employ an intermediate operator (to be identifed shortly) as an unperturbed operator. This operator is chosen close enough to the $\lambda = \infty$ operator that it may be dealt with relatively explicitly while at the same time being close enough to the operator of the original problem that a perturbation expansion can succeed. For this unperturbed operator we take

$$H_0(\lambda) = \frac{-d^2}{dx^2} + U(x) + \lambda \tilde{V}(x), \tag{3.1}$$

where $\tilde{V}(x)$ is chosen such that $\lim_{x \to 1^+} V(x)/\tilde{V}(x) = 1$. In the following we shall concern ourselves only with cases where $\tilde{V}(x) = (x-1)^p \chi_{[1,\infty)}$ (for some $p \geqq 0$) is appropriate (up to a nonzero multiplicative constant which can be absorbed into the parameter λ).

The simple scaling behavior of $\tilde{V}(x)$ allows a considerable strengthening of Corollary 2.5:

Theorem 3.1. *Given any $\lambda = \infty$ eigenvalue e, for λ large enough there is a unique eigenvalue $\tilde{E}(\lambda) = f(\lambda^{-1/(p+2)})$ of $H_0(\lambda)$ where f is an analytic function in a neighborhood of* 0 *and $f(0) = e$.*

Proof. We must show that the analytic implicit function theorem (see Theorem 2.4) applies in the present context. We shall begin by considering the case of fixed λ and then use scaling to reintroduce the parameter λ whereupon the desired result follows easily. With $\lambda = \lambda_0$ chosen sufficiently large that Lemma 2.2 applies, we obtain analyticity in E of $\psi_\infty/\psi'_\infty|_{x=1}$ where $\psi_\infty = \psi_\infty(x;E,\lambda_0)$ is a subdominant solution to $-\psi'' + \lambda_0(x-1)^p\psi = E\psi$. By a rescaling of $x-1$, we find

$$\psi_\infty(x;E,\lambda) = (\eta/\eta_0)^{1/2}\,\psi_\infty((\eta/\eta_0)^{-1}(x-1)+1;(\eta/\eta_0)^2 E,\lambda_0),$$

where $\eta = \lambda^{-1/(p+2)}$ and $\eta_0 = \lambda_0^{-1/(p+2)}$. From this it follows that

$$\frac{\psi_\infty(1;E,\lambda)}{\psi'_\infty(1;E,\lambda)} = \frac{\eta\psi_\infty(1;\eta_0^{-2}\eta^2 E,\lambda_0)}{\eta_0\psi'_\infty(1;\eta_0^{-2}\eta^2 E,\lambda_0)},$$

and analyticity in $\eta = \lambda^{-1/(p+2)}$ is an immediate consequence of the analyticity in E of $\psi_\infty(1;E,\lambda_0)/\psi'_\infty(1;E,\lambda_0)$ established previously. Hence the function F defined in (2.3) is seen to be analytic in E and η (upon noting that $\psi_0/\psi'_0|_{x=1}$ is independent of η). All other conditions needed for the analytic implicit function theorem were verified in the proof of Corollary 2.5.

Corollary 2.5 provides us with a basic "stability" result essential for our application of perturbation theory. It assures us that for λ sufficiently large the first n eigenvalues of $H(\lambda)$ and $H_0(\lambda)$ will be given precisely by the implicit functions $E_i(\lambda)$ and $\tilde{E}_i(\lambda)$ converging to $e_i (1 \leqq i \leqq n)$ as $\lambda \to \infty$. Here all eigenvalues (E_i, $\tilde{E}_i$, and e_i) are indexed according to their multiplicity which is one, since in view of the boundary condition $\psi(0) = 0$ there can be at most one linearly independent eigenfunction for any E. There is an alternative approach which proceeds from a treatment of the unperturbed operator $H_0(\lambda)$ and a direct approach to Theorem 3.1 to this stability result for eigenvalues of the perturbed operator $H(\lambda)$ by means of the min–max principle in [10].

Since $E_i(\lambda)$ and $\tilde{E}_i(\lambda)$ both converge to e_i as $\lambda \to \infty$, we may conclude that for λ sufficiently large, there exists $\varepsilon > 0$ such that $\{E \in \mathbb{C} \,|\, |E - \tilde{E}(\lambda)| < \varepsilon\} \cap \sigma(H(\lambda)) = \{E_i(\lambda)\}$ and hence that the operator

$$P_i(\lambda) = \frac{1}{2\pi i} \oint_{|E - \tilde{E}_i| = \varepsilon} (E - H(\lambda))^{-1}\, dE \tag{3.2}$$

is the one-dimensional projection operator which projects onto the eigenspace of $H(\lambda)$ corresponding to $E_i(\lambda)$. The above representation for $P_i(\lambda)$ is the key to our asymptotic expansion. We start from

$$E_i(\lambda) = \frac{(\Omega_0, H(\lambda)P_i(\lambda)\Omega_0)}{(\Omega_0, P_i(\lambda)\Omega_0)} = \tilde{E}_i(\lambda) + \frac{(\Omega_0, WP_i(\lambda)\Omega_0)}{(\Omega_0, P_i(\lambda)\Omega_0)}, \tag{3.3}$$

where Ω_0 is an eigenvector of $H_0(\lambda)$ corresponding to $\tilde{E}_i(\lambda)$ and where $W = \lambda(V - \tilde{V})$. Series expansions can now be obtained by expanding the resolvent in $P_i(\lambda)$ as a finite geometric series with remainder (which is the standard perturbation expansion approach [21]):

$$(E - H)^{-1} = \sum_{\ell=0}^{m} [(E - H_0)^{-1} W]^\ell (E - H_0)^{-1} + [(E - H_0)^{-1} W]^{m+1} (E - H)^{-1},$$

valid for all nonnegative integers m. Suppressing the index i, we have

$$E(\lambda) = \tilde{E}(\lambda) + f(\lambda)/g(\lambda), \tag{3.4}$$

where

$$f(\lambda) = (\Omega_0, WP(\lambda)\Omega_0) = \sum_{\ell=0}^{m} a_\ell + R_m(\lambda) \tag{3.5a}$$

$$g(\lambda) = (\Omega_0, P(\lambda)\Omega_0) = \sum_{\ell=0}^{m} b_\ell + S_m(\lambda), \tag{3.5b}$$

with

$$a_\ell = \frac{1}{2\pi i} \oint (E - \tilde{E})^{-1} (\Omega_0, W[(E - H_0)^{-1} W]^\ell \Omega_0) dE, \tag{3.6a}$$

$$b_\ell = \frac{1}{2\pi i} \oint (E - \tilde{E})^{-2} (\Omega_0, W[(E - H_0)^{-1} W]^{\ell-1} \Omega_0) dE, \tag{3.6b}$$

and

$$R_m(\lambda) = \frac{1}{2\pi i} \oint (\Omega_0, W[(E - H_0)^{-1} W]^{m+1} (E - H)^{-1} \Omega_0) dE, \tag{3.7a}$$

$$S_m(\lambda) = \frac{1}{2\pi i} \oint (E - \tilde{E})^{-1} (\Omega_0, W[(E - H_0)^{-1} W]^m (E - H)^{-1} \Omega_0) dE. \tag{3.7b}$$

To show that these formulae lead to an asymptotic expansion for $E(\lambda)$ we must begin by showing that the remainders R_m and S_m behave suitably. We shall do this for potentials V satisfying the conditions of case (1) with the further restriction that $V(x) = 1 + O(x - 1)$ as $x \to 1^+$. Thus our unperturbed operator (3.1) has $\tilde{V}(x) = \chi_{[1,\infty)}$ and expansion parameter $\eta = \lambda^{-1/2}$. These restrictions make it possible to find explicit expressions for the unperturbed wave-functions Ω_0 and for $(E - H_0)^{-1}$ (viewed as an integral operator with the Green function (2.4) as kernel). With such explicit representations for R_m and S_m we shall be able to estimate their orders in η. Letting $\Gamma = \{E \mid |E - \tilde{E}| = \varepsilon\}$ we have

$$|R_m| \leqq (2\pi)^{-1} \int_\Gamma |(\Omega_0, W[(E - H_0)^{-1} W]^{m+1} (E - H)^{-1} \Omega_0)| \, |dE|,$$

$$|S_m| \leqq (2\pi)^{-1} \int_\Gamma |E - \tilde{E}|^{-1} |(\Omega_0, W[(E - H_0)^{-1} W]^m (E - H)^{-1} \Omega_0)| \, |dE|,$$

and thus

$$|R_m| \leqq \varepsilon \left\{ \sup_{E \in \Gamma} \| W[(E - H_0)^{-1} W]^{m+1} \Omega_0 \| \right\} \left\{ \sup_{E \in \Gamma} \| (E - H)^{-1} \Omega_0 \| \right\},$$

$$|S_m| \leqq \left\{ \sup_{E \in \Gamma} \| W[(E - H_0)^{-1} W]^m \Omega_0 \| \right\} \left\{ \sup_{E \in \Gamma} \| (E - H)^{-1} \Omega_0 \| \right\},$$

where we have used the Schwarz inequality in obtaining the last two equations above. Since $(E - H)^{-1}$ is continuous in E and since Γ is a compact set, the second quantity in brackets above is just some constant. To obtain estimates of the order of both remainders in $\eta = \lambda^{-1/2}$ we must study the quantity $\sup_{E \in \Gamma} \| W[(E - H_0)^{-1} W]^\ell \Omega_0 \|$ for nonnegative integers ℓ. For this we shall need the following formulae ($\kappa = \sqrt{\lambda - E}$):

$$\psi_0(x) = C_0 e^{\kappa(x-1)} + D_0 e^{-\kappa(x-1)} \quad \text{for } 1 < x;$$

with

$$\begin{pmatrix} C_0 \\ D_0 \end{pmatrix} = \frac{1}{2\kappa} \begin{pmatrix} \kappa y_0(1, E) + y_0'(1, E) \\ \kappa y_0(1, E) - y_0'(1, E) \end{pmatrix};$$

$$\psi_\infty(x) = e^{-\kappa(x-1)} \quad \text{for } 1 < x;$$

and $W_{0\infty} \equiv W\{\psi_0, \psi_\infty\} = -(\kappa y_0(1, E) + y_0'(1, E))$. (This ψ_∞ has different normalization from that given by (2.2) but is slightly more convenient in the present setting.) Furthermore, we have for the unperturbed eigenfunction

$$\Omega_0(x) = y_0(1, \tilde{E})e^{-\tilde{\kappa}(x-1)} \quad \text{for } 1 < x;$$

where we use $\tilde{E}$ and $\tilde{\kappa}$ to denote values of E and $\kappa = \sqrt{\lambda - E}$ which satisfy the eigenvalue condition $\kappa y_0(1, E) + y_0'(1, E) = 0$. Note that the above information about the various functions on the exterior region $(x > 1)$ suffices for all matrix element calculations which we will encounter since the support of W is contained in this region.

We may view $\| W[(E - H_0)^{-1} W]^\ell \Omega_0 \|$ as an expression involving $\ell + 1$ integrations. After rescaling each integration variable (we replace x by $z = \eta^{-1}(x - 1)$), we factor out all identifiable factors of η and show that what remains is bounded for η sufficiently small and $E \in \Gamma$. To proceed, we need the following lemma:

Lemma 3.2. *Let $K_\pm(x, y) = e^{\pm x_<} e^{-x_>}$ on $[0, \infty) \times [0, \infty)$ and let q be continuous and such that $|q(x)| \leqq ce^{-ax}$ where a and c are positive constants. Let $r_\pm(x) = \int_0^\infty K_\pm(x, y)q(y)dy$. Then $|r_\pm(x)| \leqq \tilde{c}_\pm e^{-\tilde{a}_\pm x}$ where $\tilde{a}_\pm$ and $\tilde{c}_\pm$ are positive constants.*

Proof: First consider $r_-(x) = \int_0^\infty e^{-x_<} e^{-x_>} q(y)dy = e^{-x} \int_0^\infty e^{-y} q(y)dy$. Then $|r_-(x)| \leqq e^{-x} \int_0^\infty e^{-y}|q(y)|dy \leqq c(1 + a)^{-1} e^{-x}$. Next consider $r_+(x) = \int_0^\infty e^{x_<} e^{-x_>} q(y)dy = \int_0^\infty e^{-|x-y|}q(y)dy$. Then we have

$$\begin{aligned} |r_+(x)| &\leqq \int_0^{x/2} e^{-|x-y|}|q(y)|dy + \int_{x/2}^\infty e^{-|x-y|}|q(y)|dy \\ &\leqq e^{-x/2} \int_0^{x/2} |q(y)|dy + \int_{x/2}^\infty |q(y)|dy \\ &\leqq e^{-x/2} \int_0^\infty |q(y)|dy + ca^{-1}e^{-ax/2} \\ &\leqq ca^{-1}(e^{-x/2} + e^{-ax/2}), \end{aligned}$$

from which the conclusion to the lemma follows. □

With the help of this lemma, we can obtain the following rough estimates of R_m and S_m:

Lemma 3.3. *Let $W(x) = \lambda w(x)$ and suppose that $|w(x)| \leqq c(x - 1)e^{b(x-1)}$ on $(1, \infty)$ for some constants b and c. The remainder terms R_m and S_m are $O(\eta^{m+3/2})$ and $O(\eta^{m+1/2})$, respectively.*

Proof. We estimate $\| W[(E - H_0)^{-1} W]^\ell \Omega_0 \|$. We have

$$(W[(E - H_0)^{-1} W]^\ell \Omega_0)(x) = W(x) \int_0^\infty dx_1 G(x, x_1)W(x_1) \int_0^\infty dx_2 \ldots$$
$$\int_0^\infty dx_\ell G(x_{\ell-1}, x_\ell) W(x_\ell)\Omega_0(x_\ell) = \lambda^{\ell+1} w(x) \int_1^\infty dx_1 G(x, x_1)$$

$$\times\, w(x_1)\int_1^\infty dx_2 \ldots \int_1^\infty dx_\ell G(x_{\ell-1}, x_\ell)w(x_\ell)\Omega_0(x_\ell).$$

Hence

$$(W[(E-H_0)^{-1}W]^\ell\Omega_0)(1+\eta z) = \lambda^{\ell+1}y_0(1,\tilde{E})w(1+\eta z)\eta^\ell\int_0^\infty dz_1$$

$$\times\, G(1+\eta z, 1+\eta z_1)w(1+\eta z_1)\int_0^\infty dz_2 \ldots$$

$$\int_0^\infty dz_\ell G(1+\eta z_{\ell-1}, 1+\eta z_\ell)w(1+\eta z_\ell)e^{-\tilde{\kappa}\eta z_\ell}.$$

Now we have

$$G(1+\eta z_1, 1+\eta z_2) = W_{0\infty}^{-1}[C_0K_+(\kappa\eta z_1, \kappa\eta z_2) + D_0K_-(\kappa\eta z_1, \kappa\eta z_2)]$$

for $(z_1, z_2)\in[0,\infty)\times[0,\infty)$. We also have

$$|w(1+\eta z)| \leqq c\eta z e^{b\eta z};$$

and hence for $\tilde{w}(z) \equiv \eta^{-1}w(1+\eta z)$, we have

$$|\tilde{w}(z)| \leqq cze^{b\eta z}.$$

Therefore, $(W[(E-H_0)^{-1}W]^\ell\Omega_0)(1+\eta z)$ can be written as the sum of 2^n terms where each term has the form

$$\eta^{-2(\ell+1)}y_0(1,\tilde{E})\eta^{2\ell+1}\tilde{w}(z)\int_0^\infty dz_1K_\pm(\kappa\eta z, \kappa\eta z_1)\tilde{w}(z_1)\int_0^\infty dz_2 \ldots$$

$$\int_0^\infty dz_\ell K_\pm(\kappa\eta z_{\ell-1}, \kappa\eta z_\ell)\tilde{w}(z_\ell)e^{-\tilde{\kappa}\eta z_\ell}W_{0\infty}^{-\ell}C_0^{\#(+)}D_0^{\#(-)}.$$

Finally, since $K_\pm(\kappa\eta x, \kappa\eta y) = K_\pm(x,y)e^{\pm(\kappa\eta-1)x_<}e^{-(\kappa\eta-1)x_>}$ and $\kappa\eta = 1+o(1)$ in η we can apply Lemma 3.2 to deduce that the above n-fold integral is bounded by a decaying exponential for η sufficiently small. This leaves us with

$$|\eta^{-1}y_0(1,\tilde{E})W_{0\infty}^{-\ell}C_0^{\#(+)}D_0^{\#(-)}|\tilde{w}(z)e^{-az}$$

as a bound on a term. Hence $\|W[(E-H_0)^{-1}W]^\ell\Omega_0\|^2$ has 2^{2n} terms, where each term is bounded by a term of the form

$$|\eta^{-2}y_0^2(1,\tilde{E})W_{0\infty}^{-2\ell}C_0^{n_1}D_0^{n_2}|\int_0^\infty \eta dz|\tilde{w}(z)|^2e^{-2az}$$

$$\leqq (\text{const})\eta^{-1}y_0^2(1,\tilde{E})|W_{0\infty}^{-2\ell}C_0^{n_1}D_0^{n_2}|,$$

where n_1 and n_2 are nonnegative integers such that $n_1+n_2 = 2\ell$. To complete the proof we note that $C_0/W_{0\infty}$, $D_0/W_{0\infty}$, and $y_0(1,\tilde{E})$ are all $O(\eta)$ as η decreases to 0 and this yields

$$\|W[(E-H_0)^{-1}W]^\ell\Omega_0\| = O(\eta^{\ell+1/2}). \qquad \square$$

Next, we take a closer look at the individual terms a_ℓ and b_ℓ (3.6). By an argument like that given above the integrals defining these terms exist and a_ℓ and b_ℓ are bounded functions of η as η decreases to 0. In fact, we shall show the following:

Lemma 3.4. *Let a_ℓ and b_ℓ be defined by* (3.6). *Then $a_\ell = O(\eta^{2\ell+2})$ and $b_\ell = O(\eta^{2\ell})$.*

Proof. We shall only sketch how one must modify the proof of Lemma 3.3 to obtain the above result. Here one does not bound the integral using the Schwarz inequality but rather one attempts an exact evaluation of the integral using the calculus of residues. The Wronskian $W_{0\infty}$ has $\tilde{E}$ as an isolated simple root so one must calculate derivatives at $E = \tilde{E}$. With each derivative one finds an associated η^2. These together with the η's which appear as before combine to produce the stated behavior with respect to η.

We combine Lemmas 3.3 and 3.4 to obtain our next theorem.

Theorem 3.5. *Suppose $V(x) = 1 + O(x-1)$ as $x \to 1^+$ and that V is exponentially bounded at infinity. Then $E(\lambda) = \tilde{E}(\lambda) + h(\lambda)$, where $h(\lambda) = \sum_{\ell=0}^{m} c_\ell + T_m(\lambda)$ for each nonnegative integer m and where $c_\ell = O(\eta^{2\ell+2})$ and $T_m = O(\eta^{2\ell+4})$. Furthermore, the c_ℓ's may be obtained from $\sum_{\ell=0}^{m} c_\ell b_{m-\ell} = a_m, m = 0, 1, 2, \ldots$.*

Proof. First let us consider the function f of (3.5a) (g is treated analogously). From $R_m = \sum_{\ell=m+1}^{2m+3} a_\ell + R_{2m+3}$ we see that $R_m = O(\eta^{2m+4})$. Similarly, $S_m = O(\eta^{2m+2})$. With these improved estimates of the remainders R_m and S_m and the fact that $b_0 = (\Omega_0, \Omega_0) \neq 0$, it is a routine matter to verify the conclusions of the theorem. □

To guarantee a true power series expansion in η for $E(\lambda)$, we need to place further conditions on $V(x)$. Specifically, we shall assume that $V(x)$ itself has an asymptotic power series in $x-1$ as $x \to 1^+$:

$$V(x) \sim 1 + \sum_{m=1}^{\infty} \alpha_m (x-1)^m \qquad \text{as } x \to 1^+. \tag{3.8}$$

Then we have:

Theorem 3.6. *Suppose that $V(x)$ satisfies* (3.8) *and that V is exponentially bounded at infinity. Then $E(\lambda)$ has an asymptotic power series expansion in η,*

$$E(\lambda) \sim \sum_{m=0}^{\infty} \beta_m \eta^m,$$

and the β_m depend on V only through the coefficients α_m.

Proof. The proof of this theorem rests on showing that the terms a_ℓ and b_ℓ (3.6) have asymptotic power series expansions in η. This result follows from a series of technical lemmas which will conclude this section. If we assume that it holds for the time being we can easily show that f and g have asymptotic power series expansions in η. (To any finite order one only has to deal with a finite number of terms in powers of η and a finite number of remainders.) Finally, the construction of asymptotic power series for $h = f/g$ and then for $\tilde{E} + h$ follows the patterns already set.

The lemmas which allow us to expand the terms a_ℓ and b_ℓ in powers of η take their inspiration from Watson's Lemma. This lemma tells us that if $g(x) \sim \sum_{n=0}^{\infty} \gamma_n x^n$ and g is exponentially bounded (i.e. $|g(x)| \leqq Ae^{ax}$ for some constants A, $a > 0$) then $\int_0^\infty e^{-x} g(\eta x)dx \sim \sum_{n=0}^{\infty} \gamma_n \left(\int_0^\infty e^{-x} x^n dx \right) \eta^n = \sum_{n=0}^{\infty} n!\gamma_n \eta^n$. First, we prove a slightly more general version of Watson's Lemma:

Lemma 3.7. *Suppose that $f(x, \eta)$ obeys the following conditions:*

(*i*) $|f(x,\eta)| \leqq Ae^{a\eta x}$ *for all* $x \in [0, \infty)$ *and for* η *sufficiently small.*

(*ii*) $f(x,\eta) \sim \sum_{n=0}^{\infty} g_n(x)\eta^n$ *as* $\eta \to 0^+$, *where* $g_n(x)$ *is a polynomial for each* n.

(*iii*) *For each* N *there exists* $\delta > 0$ *such that the* N^{th} *remainder* $R_N(x,\eta) = f(x,\eta) - \sum_{n=0}^{N} g_n(x)\eta^n$ *satisfies* $|R_N(x,\eta)| \leqq p_N(x)\eta^{N+1}$ *for any fixed* $x \in [0, \infty)$ *and for all* $\eta \in (0, \delta/x)$, *with* p_N *a polynomial.*

Let $\tilde{f}(\eta) = \int_0^\infty e^{-x} f(x,\eta)dx$. *Then* $\tilde{f}(\eta) \sim \sum_{n=0}^{\infty} \left(\int_0^\infty e^{-x} g_n(x)dx \right) \eta^n$.

Proof. We wish to show that $\tilde{R}_N(\eta) \equiv \tilde{f}(\eta) - \sum_{n=0}^{N} \left(\int_0^\infty e^{-x} g_n(x)dx \right) \eta^n$ is $O(\eta^{N+1})$. We have $\tilde{R}_N(\eta) = \int_0^\infty e^{-x} R_N(x,\eta)dx$ and hence

$$|\tilde{R}(\eta)| \leqq \int_0^{\delta/\eta} e^{-x} p_N(x)\eta^{N+1} dx + \int_{\delta/\eta}^{\infty} e^{-x} |R_N(x,\eta)| dx.$$

Now the first integral is bounded by $\eta^{N+1} \int_0^\infty e^{-x} p_N(x)dx = O(\eta^{N+1})$ and the second can be shown to be $O(e^{-\tilde{\delta}/\eta})$ (one substitutes $R_N(x,\eta) = f(x,\eta) - \sum_{n=0}^{N} g_n(x)\eta^n$ and then makes use of condition (i)) where $\tilde{\delta} \in (0, \delta)$. Hence $\tilde{R}_N(\eta) = O(\eta^{N+1})$ and we are done. $\square$

Next, we present a lemma whose proof is even more straightforward:

Lemma 3.8. *Suppose that* $f(x,\eta)$ *obeys conditions* (i)–(iii) *of Lemma* 3.7. *Let* $\tilde{f}(x,\eta) \equiv \eta \int_0^x f(y,\eta)dy$. *Then* $\tilde{f}(x,\eta) \sim \sum_{n=1}^{\infty} \left(\int_0^x g_{n-1}(y)dy \right) \eta^n$ *and furthermore* $\tilde{f}(x,\eta)$ *obeys conditions* (i)–(iii) (*with other choices of constants and polynomials perhaps*).

Proof. We have $\tilde{R}_N(x,\eta) = \tilde{f}(x,\eta) - \sum_{n=1}^{N} \left(\int_0^x g_{n-1}(y)dy \right) \eta^n = \eta \int_0^x R_{N-1}(y,\eta)dy$. Hence

$$|\tilde{R}_N(x,\eta)| \leqq \left(\int_0^x p_{N-1}(y)dy \right) \eta^{N+1}$$

for $\eta \in (0, \delta/x)$ and therefore $\tilde{R}_N(x,\eta)$ obeys condition (iii). This and the observation that $\int_0^x g_n(y)dy$ is a polynomial yields condition (ii). To verify condition (i) we take

$$|\tilde{f}(x,\eta)| \leqq \eta \int_0^x |f(y,\eta)|dy \leqq A\eta \int_0^x e^{a\eta y}dy = Aa^{-1}(e^{a\eta x}-1) \leqq Aa^{-1}e^{a\eta x}. \qquad \square$$

There is one other lemma which we shall need:

Lemma 3.9. *Suppose that* $f(x,\eta)$ *obeys conditions* (i)–(iii) *of Lemma* 3.7. *Let* $\tilde{f}(x,\eta) = e^x \int_x^\infty e^{-y} f(y,\eta)dy$. *Then* $f(x,\eta) \sim \sum_{n=0}^{\infty} \left(e^x \int_x^\infty e^{-y} g_n(y)dy \right)\eta^n$ *and furthermore* $\tilde{f}(x,\eta)$ *obeys conditions* (i)–(iii).

Proof. $\tilde{R}_N(x,\eta) = \tilde{f}(x,\eta) - \sum_{n=0}^{N} \left(e^x \int_x^\infty e^{-y} g_n(y)dy \right)\eta^n = e^x \int_x^\infty e^{-y} R_N(y,\eta)dy$. Thus $|\tilde{R}_N(x,\eta)| \leqq e^x \int_x^{\delta/\eta} e^{-y} p_N(y)\eta^{N+1}dy + e^x \int_{\delta/\eta}^{\infty} e^{-y}|R_N(y,\eta)|dy$, and as in the proof of Lemma 3.7 the second integral is exponentially small in η. If we transform to $u = y - x$ in the first integral, we obtain $e^x \int_x^{\delta/\eta} e^{-y} p_N(y)\eta^{N+1}dy \leqq e^x \int_x^\infty e^{-y} p_N(y)\eta^{N+1} dy = \left(\int_0^\infty e^{-u} p_N(x+u)du \right)\eta^{N+1}$. Noting that $\int_0^\infty e^{-u} p_N(x+u)du$ is a polynomial in x, we see that $\tilde{R}(x,\eta)$ obeys condition (iii). Likewise $e^x \int_x^\infty e^{-y} g_n(y)dy$ is a polynomial and condition (ii) holds. Lastly,

$$|\tilde{f}(x,\eta)| \leqq e^x \int_x^\infty e^{-y}|f(y,\eta)|dy \leqq Ae^x \int_x^\infty e^{-y}e^{a\eta y}dy = A(1-a\eta)^{-1}e^{a\eta x} \leqq 2Ae^{a\eta x}$$

for η sufficiently small and thus condition (i) is also satisfied. $\square$

The three preceding lemmas together with an induction argument are all that is needed to obtain asymptotic power series for a_ℓ and b_ℓ. Lemma 3.7 is needed to handle integrals of $K_-(x,y)$ over $[0,\infty)$, Lemma 3.8 is needed to handle integrals of $K_+(x,y)$ over $[0,x]$, and Lemma 3.9 is needed to handle integrals of $K_+(x,y)$ over $[x,\infty)$. To start the induction, we must show that $e^{\pm(\kappa\eta-1)y}\tilde{w}(y)e^{-(\tilde{\kappa}\eta-1)y}$ satisfies conditions (i)–(iii) of Lemma 3.7. These conditions follow in a straightforward fashion once one notes that $\kappa\eta - 1 = O(\eta^2)$.

Remarks. (1) Lemmas 3.7–9 and induction give an asymptotic series for the matrix elements contained in a_ℓ and b_ℓ. We complete the argument by recalling that asymptotic series remain valid when integrated with respect to a parameter [22]. While one might be tempted to count leading powers through the induction process, we point out that the contour integral over E might very well lead to a wholesale vanishing of terms (as in the case of $b_1 = 0$).

(2) There is no reason to suspect that a result similar to Theorem III.6 (with $\eta = \lambda^{-1/(p+2)}$) would not hold for a potential V having leading behavior at 1 like $(x-1)^p$, p a positive integer. However, technical complications arise when one tries to obtain the analogues of Lemmas 3.7–9 in these cases.

(3) The hypothesis concerning the exponential boundedness of V is also of a purely technical nature. If one included in $H_0(\lambda)$ terms from the asymptotic expansion of V through order q (where $(x-1)^q$ has a positive coefficient), it should in principle be possible to allow V to grow as fast as $\exp(cx^{q/2+1})$ at infinity (c arbitrary). The only impediments to obtaining such a result are again the technical difficulties inherent in generalizing Lemmas 3.7–9.

Note. Motivated by the results presented here, B. Simon has succedded in proving "stability" results for embedded Dirichlet eigenvalues in the fully n-dimensional case. These results will appear in B. Simon, "Exterior Complex Scaling and Molecular Resonances in the Born–Oppenheimer Approximation."

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